

The Thomas-Fermi and the Thomas-Fermi-Dirac Model in Two-Dimension-  
the Effect of Strong Magnetic Field

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We have studied the properties of electron gas in two-dimension (2D) in presence of a strong orthogonal quantizing magnetic field inside a 2D Wigner-Seitz (WS) cell using Thomas-Fermi model. The electron-electron Coulomb exchange interaction in quasi-2D case is obtained. The exact form of exchange term in 2D is then derived making the width of the system tending to zero. The exchange term is then used to obtain the Thomas-Fermi-Dirac equation in 2D. We have noticed that only the ionized WS cell can have finite radius in the Thomas-Fermi model, even in presence of a strong quantizing magnetic field. On the other hand, in the Thomas-Fermi-Dirac model a neutral WS cell can have finite radius.

# 1 Introduction

Using Fermi statistics, a formalism was developed by L.H. Thomas and E. Fermi to obtain the charge distribution and also the distribution of electric field in the extra-nuclear space inside heavy atoms [1, 2]. This proposed formalism is the so called Thomas-Fermi model. The electrons inside the atoms are assumed to be a degenerate Fermi gas. In this model the electron density is found to be nonuniform inside the atom, i.e.,  $n_e = n_e(\vec{r})$ , where  $\vec{r}$  is the radial distance vector of the point from the nucleus situated at the center of the atom. The electric potential  $\phi(\vec{r})$  and the corresponding electric field  $\vec{E}(\vec{r})$  within the atom also vary with the radial distance. The electron density has been observed to be a smoothly varying function of radial coordinate  $r$  (the atoms are assumed to be of spherical in shape), instead of having peaks according to shell model. The model was successful in predicting the binding energies of the atoms [3]. With some suitable modification the model has been successfully applied to molecules, solids and also to nuclei [4] to explain some of the experimental values. The electronic shell effect was also incorporated in the model. The model could also satisfactorily explain the thermodynamic properties of dense degenerate electron gas. For very high density matter, the electron gas surrounding the nucleus is assumed to be enclosed in a region, called WS cell [5]. Therefore in such situation, instead of atoms, there are regularly spaced WS cells, which are assumed to be charge neutral and spherically symmetric. There are also relativistic generalization of TF model for very high energy electron gas and the model was found to be successfully to investigate the thermodynamic properties of such igh density degenerate electron gas[8].

Generalized versions of non-relativistic as well as relativistic form of Thomas-Fermi equations in presence of strong quantizing magnetic field, when the Landau levels for the electrons are populated have also been obtained [7, 9, 10]. The thermodynamic properties of matter inside the magnetically deformed WS cells have also been investigated. In presence of strong quantizing magnetic field, the electron pressure becomes anisotropic inside the WS cells. As a result they will be deformed to ellipsoidal shape from their usual spherical structure [11].

However, all these investigations are associated with the three dimensional degenerate electron gas, enclosed inside the WS cells. There are only a few reported results on the study of two dimensional electron gas using Thomas-Fermi model [12, 13, 14]. Further, to the best of our knowledge,

no studies have been reported on the two dimensional Thomas-Fermi model for electron gas in presence of strong quantizing orthogonal magnetic field, in which the Landau levels are populated for the electrons. Again, in the three dimensional case, incorporating electron-electron exchange interaction, a modified form of Thomas-Fermi equation, called Thomas-Fermi-Dirac equation has been developed both for non-relativistic as well as relativistic electron gas with or without the presence of magnetic field [5, 6, 7, 8, 9]. Unfortunately, no such formalism has been developed in the case of two dimension. To the best of our knowledge, the first reported result on two dimensional Thomas-Fermi model for degenerate electron gas is by Bhaduri et. al. [12] (see also [13, 14]).

Two dimensional electron gas has a lot of important applications in modern days condensed matter physics. The electrons in 2D are constrained to move in two dimensional sheet embedded in a three dimensional space. Such two dimensional electron gas may be realized in many semi-conductor devices [15]. There are also possibility of having two dimensional electron gas on the surface of materials, e.g., liquid He [16]. In such system electrons are free to move on the surface of liquid He but rigidly attached with the He atoms. There are also a kind of solid insulators, e.g., topological insulators [17], the surface of which supports conducting states of free electrons.

During the present days the most interesting two dimensional system in condensed matter physics is the so called graphene. It is an almost ideal two dimensional material developed in the laboratory using graphite [18, 19, 20]. It has also been observed that the graphene can also support 2-D electron gas. This has become a topic of current interest due to a large number of application of graphene. There are also a lot of academic interest to study graphene theoretically. In particular application of quantum electrodynamics and the study of the physics of mass-less electrons or chiral electrons using two component Dirac equation.

In the present article we have investigated the properties of electron gas enclosed in two-dimensional WS cells, which are embedded in a three-dimensional space. The WS cell is assumed to be in  $x - y$  plane and the strong magnetic field is along  $z$ -axis. The electrons are constrained to move on  $x - y$  plane. The presence of strong magnetic field along  $z$ -direction makes electron energy eigen value discrete. The motion of the electrons on  $x - y$  plane are in quantized form. This is the well known Landau quantization in 2D. The electron energy therefore does not depend on  $p_z$ , the component of momentum along  $z$ -direction. however, the momentum component on  $x - y$

plane changes in a discrete manner.

We have organized various sections of this article in the following manner: In the next section we have developed the basic formalism for two dimensional Thomas-Fermi model for degenerate electron gas in presence of strong quantizing orthogonal magnetic field. In section 3 we have studied the thermodynamic properties of 2D degenerate electron gas inside a WS cell in presence of a strong quantizing magnetic field. In section 4 we have considered the electron-electron exchange interaction in absence of magnetic field and incorporate this result in Thomas-Fermi condition to obtain Thomas-Fermi-Dirac equation satisfied by degenerate electron gas in 2D. In section 5 we have shown explicitly that the same technique can not be followed to obtained Thomas-Fermi-Dirac equation for degenerate electron gas in presence of strong quatizing magnetic field. However, for the conventional three dimensional case, one can obtain exchange energy for electrons [9]. Finally we present the conclusion of this work.

## 2 Basic Formalism

We assume that the constant external magnetic field  $\vec{B}$  is along z-direction. In presence of this strong external quantizing magnetic field, the Landau levels of the electrons are populated on x-y plane. Since the electrons are constrained to move on x-y plane, the momentum component along z-direction,  $p_z = 0$ . The quantized form of electron energy eigen value is then given by  $\varepsilon_n = (n + \frac{1}{2})\hbar\omega$ , where  $\omega = eB/mc$ , the cyclotron frequency and  $n = 0, 1, 2, \dots, n_{max}$ , the Landau quantum numbers,  $n_{max}$  is the upper limit of Landau quantum number which is finite if the temperature of the system is zero or less than the corresponding Fermi temperature, whereas,  $n_{max} = \infty$  if the electron gas is at non zero temperature. Therefore  $n_{max}$  is finite for strongly degenerate electron gas, whereas in the non-degenerate scenario,  $n_{max}$  is infinitely large. In the strong degenerate condition the number of electrons per unit surface area is given by

$$n_e = \frac{eB}{2\pi^2} (n_{max} + 1) \quad (1)$$

Assuming  $\varepsilon_F = (n_{max} + \frac{1}{2})\hbar\omega$  as the Fermi energy of the system, we have in natural units ( $\hbar = c = 1$ ),

$$n_{max} = \frac{\varepsilon_F}{\omega} - \frac{1}{2}$$

Then

$$n_e = \frac{eB}{\pi^2} \left( \frac{\varepsilon_F}{\omega} + \frac{1}{2} \right) \quad (2)$$

Now we assume that for such degenerate electron gas confined inside a 2D WS cell, at the centre of which there are nuclei with charge  $Ze$  and the total charge carried by the electrons is  $-eN$ . Since both the protons inside the nucleus and the electrons within the WS cell carry electric charges, the Poisson's equation satisfied by the electrostatic potential  $\phi$ , produced jointly by the electrons and protons is given by

$$\nabla^2 \phi = 2\pi e n_e - 2\pi Z e \delta(r) \quad (3)$$

Here the nucleus is assumed to be a point object. The Thomas-Fermi condition in this particular situation is given by

$$\mu = \varepsilon_F = \left( n_{max}(r) + \frac{1}{2} \right) \omega - e\phi(r) = \text{constant} \quad (4)$$

which gives

$$n_{max}(r) = \frac{\mu + e\phi(r)}{\omega} - \frac{1}{2} \quad (5)$$

The number of electrons per unit surface area is then given by

$$n_e(r) = \frac{eB}{2\pi^2} (n_{max}(r) + 1) = \frac{eB}{2\pi^2} \left( \frac{\mu + e\phi(r)}{\omega} + \frac{1}{2} \right) \quad (6)$$

Since  $\phi$  is a function of radial coordinate  $r$ , both  $n_e$  and  $n_{max}$  should also depend on the radial coordinate. Here for the sake of simplicity we assume circular symmetry for the WS cells. The above mentioned variables therefore do not depend on the angular coordinate  $\theta$ . Then from the above equation we have in the extra-nuclear space of WS cell

$$\nabla^2 \phi = \frac{2\pi^2 \omega}{e^2 B} \nabla^2 n_e \quad (7)$$

and from the Poisson's equation (eqn.(3)) we have

$$\frac{2\pi^2 \omega}{e^2 B} \nabla^2 n_e = 2\pi n_e e \quad (8)$$

This a second order differential equation for the electron density  $n_e$ . On substituting the value of cyclotron frequency, eqn.(8) can be re-expressed as

$$\nabla^2 n_e = \frac{e^2}{\pi} m n_e \quad (9)$$

Hence for the 2D case, with circular symmetry, the Poisson's equation in radial coordinate  $r$  is given by

$$\frac{d^2 n_e}{dr^2} + \frac{1}{r} \frac{dn_e}{dr} = \frac{e^2 m}{\pi} n_e \quad (10)$$

Defining the scaled radius parameter  $x$ , given by

$$r = \left(\frac{\pi}{e^2 m}\right)^{1/2} x = bx, \quad (11)$$

we have

$$\frac{d^2 n_e}{dx^2} + \frac{1}{x} \frac{dn_e}{dx} - n_e = 0 \quad (12)$$

Which is the Thomas-Fermi equation in 2D in presence of a strong orthogonal quantizing magnetic field. The form of this equation is identical with that of field free case [12], except the scaling parameter  $b = (\pi/e^2 m)^{1/2}$ . Surprisingly the radius of the circular type WS cell does not change with the strength of magnetic field. However, in the usual three dimensional case, the radius of the spherical type WS cell decreases with the strength of magnetic field, e.g., in [9, 10] the scaling parameter  $\mu = (\pi/2e^3 B)^{1/2}$ , hence the actual radius  $r = \mu x$  varies with magnetic field in the form  $1/B^{1/2}$ . In the case of magnetically deformed cylindrical type WS cell, both the radial as well as the axial parameters decrease with the strength of magnetic field [11]. Therefore we can conclude that in 2D there will be no magnetic contraction of WS cells and due to the circular geometrical structure, even in presence of ultra strong quantizing magnetic field, there will be no magnetic distortion to elliptical shape. Now it is trivial to show that the general solution of eqn.(12) is given by [21]

$$n_e(x) = AI_0(x) + BK_0(x) \quad (13)$$

where  $A$  and  $B$  are two unknown constants to be obtained from the initial and the boundary conditions and can be expressed in terms of  $x_s$ , the surface value of  $x$ ,  $N$ , the total number of electrons in the system and  $Z$ , the total positive charge within the nucleus situated at the centre of the WS cell.

From the above solution it is quite obvious that  $\phi(x) \rightarrow \infty$  as  $x \rightarrow 0$  from the diverging nature of the modified Bessel function  $K_0(x)$  ( $K_0(x) \sim -\ln x$  as  $x \rightarrow 0$ ). This is also true in the case of three dimensional Thomas-Fermi equation, having a singular nature at the origin. The special technique developed by Fermi, Metropolis and Teller [22] is used to solved the Thomas-Fermi differential equation in the three dimensional case. Now the constant chemical potential for the electrons inside the WS cells is given by

$$\mu = 2\pi^2 m n_e(x) - e\phi(x) - \frac{eBm}{2} \quad (14)$$

This is the so called 2D version of Thomas-Fermi condition. For  $x = 0$

$$e\phi(0) = -\mu + 2\pi^2 m n_e(0) - \frac{eBm}{2} \quad (15)$$

and for  $x = x_s$ , i.e. at the surface  $n_e(x_s) = 0$ , therefore

$$e\phi(x_s) = \mu + \frac{eBm}{2} \quad (16)$$

Now in 2D, the potential is given by

$$e\phi(r) = -Ze^2 \ln\left(\frac{r}{a}\right) + e^2 \int n(r) \ln\left(\frac{|r - r'|}{a}\right) d^2r \quad (17)$$

Here  $e^2$  has the dimension of energy. In terms of scaled radial parameter  $x$  the above equation becomes

$$e\phi(x) = -Ze^2 \ln x + e^2 b^2 \int n(x') \ln |x - x'| d^2x' - e^2(N - Z) \ln\left(\frac{b}{a}\right) \quad (18)$$

Following [12], we have

$$\begin{aligned} e\phi(x) &= -Ze^2 \ln x + 2\pi e^2 b^2 \left( \ln x \int_0^x x' n(x') dx' + \int_x^{x_s} x' \ln x' n(x') dx' \right) \\ &- (Z - N)e^2 \ln\left(\frac{b}{a}\right) \end{aligned} \quad (19)$$

Hence for  $x > x_s$

$$e\phi(x) = -(Z - N)e^2 \left( \ln x + \ln\left(\frac{a}{b}\right) \right) \quad (20)$$

and

$$\mu = e\phi(x_s) - \frac{eBm}{2} = -(Z - N)e^2 \left( \ln x_s + \ln \left( \frac{b}{a} \right) \right) - \frac{eBm}{2} \quad (21)$$

further

$$\begin{aligned} e\phi(0) = -Ze^2 \ln x \big|_{x \rightarrow 0} &+ 2\pi e^2 b^2 \int_0^{x_s} x \ln x n(x) dx \\ &+ (N - Z)e^2 \ln \left( \frac{b}{a} \right) \end{aligned} \quad (22)$$

which is also given by

$$\begin{aligned} \mu - 2\pi^2 mn(x_s) + \frac{eBm}{2} &= -(Z - N)e^2 \left( \ln x_s + \ln \left( \frac{b}{a} \right) \right) \\ - \frac{eBm}{2} - 2\pi^2 mn(x_s) + \frac{eBm}{2} &= -Ze^2 \ln x \big|_{x \rightarrow 0} \\ + 2\pi e^2 b^2 \int_0^{x_s} x \ln x n(x) dx &+ (N - Z)e^2 \ln \left( \frac{b}{a} \right) \end{aligned} \quad (23)$$

Combining eqn.(22) and eqn(23), we finally get

$$e^2(N - Z) \ln x_s = 2\pi e^2 b^2 \int_0^{x_s} x \ln x n(x) dx \quad (24)$$

Since  $n(x_s) = 0$ , we have

$$AI_0(x_s) + BK_0(x_s) = 0 \quad (25)$$

and

$$x_s n'(x_s) = \frac{(N - Z)}{2\pi b^2} \quad (26)$$

The right hand side of eqn.(26) vanishes for  $N = Z$ , i.e., for a charge neutral two dimensional WS cell. Hence from the relations  $I'_0(x) = I_1(x)$  and  $K'_0(x) = -K_1(x)$ , we get

$$A = B \frac{K_1(x_0)}{I_1(x_0)} \quad (27)$$

Now using the relation

$$2\pi b^2 \int_0^{x_s} x n(x) dx = N \quad (28)$$



and from the integrals of  $K_0(x)$  and  $I_0(x)$  [21], we have

$$x_s[AI_1(x_s) - BK_1(x_s)] = x_s n'(x_s) = \left( \frac{N}{2\pi b^2} - B \right) \quad (29)$$

Hence we can write

$$B = \frac{Z}{2\pi b^2} \quad (30)$$

Further using the Wronskian

$$I_\nu(x)K_{\nu+1}(x) + I_{\nu+1}(x)K_\nu(x) = \frac{1}{x} \quad (31)$$

we have

$$I_0(x) = \frac{Z}{Z - N} \quad (32)$$

It is quite obvious from eqn.(32) that for  $N = Z$ , the radius of the WS cell is infinitely large. It is also to be noted further that for the finite value of the radius parameter  $x$ ,  $N$  should be less than  $Z$ , i.e., the cell must be in ionized state with net positive charge. In fig.(1) we have plotted the variation of the value of  $x_s$ , the scaled radius parameter with  $N/Z$ .

### 3 Thermodynamic of 2D Electron Gas

The expressions for internal energy density and the corresponding kinetic pressure can be obtained from the first principle as has been followed in basic statistical mechanics. We define the  $q$ -potential of Kramers in the form [23]

$$q = \frac{PS}{kT} = \sum_i \ln[1 + \exp(-\alpha' - \beta\varepsilon_i)] \quad (33)$$

where  $P$  is the kinetic pressure,  $S$  is the surface area,  $T$  is the temperature of the system,  $k$  is the Boltzmann constant,  $\alpha' = \alpha - \beta e\phi$ ,  $\alpha = -\mu/kT$ , with  $\mu$ , the chemical potential of the electrons and  $\beta = 1/kT$ . In presence of a strong orthogonal quantizing magnetic field, which populates the electron Landau levels, the energy eigen value corresponding to  $n$ th. Landau level is given by  $\varepsilon_n = (n + \frac{1}{2})\hbar\omega = (n + \frac{1}{2})\omega$  for  $\hbar = 1$ . The total kinetic energy of the electron gas is then given by

$$E = \left( \frac{\partial q}{\partial \beta} \right)_{\alpha, S} = \frac{eBS}{2\pi^2} \sum_{n=0}^{\infty} \frac{\varepsilon_n}{\exp[\beta(\varepsilon_n - \mu')] + 1} \quad (34)$$

where  $\mu' = \mu + e\phi$ . For degenerate case, since the Fermi distribution function reduces to unity, we have

$$E = \frac{eBS}{2\pi^2} \sum_{n=0}^{n_{max}} \left(n + \frac{1}{2}\right) \omega \quad (35)$$

On summing over  $n$  we can express the surface density of electron kinetic energy in the form

$$\epsilon(x) = \frac{e^2 B^2}{4\pi^2 m} (n_{max}(x) + 1)^2 \quad (36)$$

The kinetic pressure can also be obtained from  $q$ -potential. Using the Euler summation formula (discussed in the Appendix) the degeneracy pressure for electron gas in 2D is given by

$$P(x) = \frac{m}{4\pi^2} (\mu + e\phi(x))^2 = \frac{e^2 B^2}{4\pi^2 m} \left(n_{max}(x) + \frac{1}{2}\right)^2 \quad (37)$$

## 4 Electron Exchange Energy for $B = 0$

we shall now obtain the electron exchange energy (see [5] for three-dimensional case). For the sake of simplicity we start with an ideal two-dimensional system of degenerate electron gas. In the case of a purely two-dimensional electron gas, the electron-electron two body potential is logarithmic in nature and may be expressed in the form

$$V_{ee} = e^2 \ln \left( \frac{|\vec{r} - \vec{r}'|}{a} \right) \quad (38)$$

where as stated before,  $e^2$  has the dimension of energy. In 2D, the normalized form of free electron wave functions are given by

$$\psi(\vec{r}) = \frac{1}{S^{\frac{1}{2}}} \exp(i\vec{k} \cdot \vec{r}) \quad (39)$$

Then the exchange part of interaction may be written as

$$U_{ex}(\vec{r})\psi_i(\vec{r}) = \sum_{j=1}^N \psi_j(\vec{r}) \int \psi_j^*(\vec{r}') V(|\vec{r} - \vec{r}'|) \psi_i(\vec{r}') d^2 r' \quad (40)$$

which after some straight forward algebra may be expressed in the form

$$U_{ex}(\vec{r})\psi_i(\vec{r}) = \frac{e^2}{S^{\frac{3}{2}}} \sum_j \exp(i\vec{k} \cdot \vec{r}) \int \exp(i(\vec{k} - \vec{k}') \cdot (\vec{r}' - \vec{r})) V(|\vec{r} - \vec{r}'|) d^2r' \quad (41)$$

Hence the expectation value for the electron exchange energy is given by

$$U_{ex} = \frac{e^2}{S} \sum_j \int \exp(i\vec{K} \cdot \vec{s}) V(s) d^2s \quad (42)$$

where  $\vec{K} = \vec{k} - \vec{k}'$ ,  $\vec{s} = \vec{r} - \vec{r}'$  and  $d^2s = s ds d\theta$ . Then the angular part of the integral is given by

$$\int_0^{2\pi} \exp(iKs \cos \theta) d\theta \quad (43)$$

Now to evaluate this angular integral we use the following trivial algebraic relation

$$\exp(iks \cos \theta) = \cos(ks \cos \theta) + i \sin(ks \cos \theta) \quad (44)$$

And use the standard relations [21]

$$\cos(z \cos \theta) = J_0(z) + 2 \sum_{k=1}^{\infty} (-1)^k J_{2k}(z) \cos(2k\theta) \quad (45)$$

and

$$\sin(z \cos \theta) = 2 \sum_{k=0}^{\infty} (-1)^k J_{2k+1}(z) \cos(2k\theta) \quad (46)$$

where  $J_n(z)$  is the ordinary Bessel function of order  $n$ . Then after some straight forward algebra we have the exchange interaction part

$$U_{ex} = \frac{2\pi e^2}{S} \sum_j \int s ds J_0(ks) V(s) = \frac{2\pi e^2}{(2\pi)^2} \int d^2k' \int s ds J_0(ks) V(s) \quad (47)$$

where we have used the relation  $\frac{1}{S} \sum_j \longrightarrow \frac{1}{(2\pi)^2} \int d^2k'$ . The integral as given by eqn.(47) is obviously a diverging one for logarithmic form of  $e-e$  coulomb potential as given in eqn.(38). The coulomb exchange energy therefore has infinite contribution in the case of ideal 2D electron gas, which is totally unphysical in nature. Hence, to obtain a finite contribution of exchange part of  $e-e$  interaction energy, we therefore follow an alternative approach. Instead

of an ideal two-dimensional system, we consider a quasi two dimensional degenerate electron gas with an width  $\Delta z$  along the third dimension and we shall make it tending to zero at the end [24]. The wave functions in the  $x-y$  plane is as usual are given by eqn.(39), with  $\vec{r}$  replaced by  $x$  and  $y$ . In the  $z$ -direction the wave function is assumed to be given by

$$\phi_0(z) = \frac{1}{(\Delta z)^{\frac{1}{2}}} \cos\left(\frac{\pi z}{\Delta z}\right) \quad (48)$$

Then following [24] (see also [25]), we have for the limiting case  $\Delta z \rightarrow 0$ ,

$$U_{ex} = -\frac{4}{3\pi}(2\pi n_e)^{\frac{1}{2}} \quad (49)$$

where  $n_e = k_F^2/2\pi$ . The modified form of Thomas-Fermi condition is then given by

$$\mu = \frac{k_f^2}{2m} - e\phi - \frac{4}{3}\left(\frac{2}{\pi}\right)^{\frac{1}{2}} n_e^{\frac{1}{2}} \quad (50)$$

Which is the Thomas-Fermi-Dirac condition in 2D scenario. Hence

$$k_F = \frac{4m}{3\pi} + m\left(\frac{16}{9\pi^2} + \frac{2}{m}(\mu + e\phi)\right)^{1/2} \quad (51)$$

the other solution for Fermi momentum has been discarded for obvious reason. Let us now substitute

$$\frac{8m}{9\pi^2} + (\mu + e\phi) = \frac{Ze^2}{r}\omega(r), \quad (52)$$

then we have from eqn.(51)

$$k_F = \frac{4\pi}{3m} + (2m)^{\frac{1}{2}} \frac{Z^{\frac{1}{2}}e}{r^{\frac{1}{2}}} \omega^{\frac{1}{2}} \quad (53)$$

Hence from the Poisson's equation we can write down the Thomas-Fermi-Dirac equation in the following form

$$r^2 \frac{d^2\omega}{dr^2} - r \frac{d\omega}{dr} + \omega = r^3 2me^2 \left[ \frac{\omega^{1/2}}{r^{1/2}} + \frac{4\pi}{3m} \frac{1}{(2mZe^2)^{\frac{1}{2}}} \right]^2 \quad (54)$$

Writing  $r = ax$ , with  $x$ , the dimensionless radius parameter and  $a$  is an unknown constant, the above equation can be expressed in the following form:

$$x^2 \frac{d^2 \omega}{dx^2} - x \frac{d\omega}{dx} + \omega = x^3 \left[ \frac{\omega^{\frac{1}{2}}}{x^{\frac{1}{2}}} + \alpha \right]^2 \quad (55)$$

with

$$a = (2me^2)^{-\frac{1}{2}} \quad \text{and} \quad \alpha = \frac{4\pi}{3m} \left[ \frac{1}{Z(2me^2)^{\frac{3}{2}}} \right]^{\frac{1}{2}} \quad (56)$$

The complementary function can be obtained from the solution of the equation

$$x^2 \frac{d^2 \omega}{dx^2} - x \frac{d\omega}{dx} + \omega = 0 \quad (57)$$

To get an analytical solution, we put  $x = \exp(z)$ , with  $-\infty \leq z \leq z_s$ , where  $z_s$  corresponds to surface value. Hence we have

$$(D^2 - 2D + 1)\omega(z) = 0 \quad (58)$$

where  $D = d/dz$ . The solution of this equation, which is the complementary function is then given by

$$\omega = (A + Bz) \exp(z) + 1 \quad (59)$$

where  $A$  and  $B$  are two unknown constants. The factor 1 is put by hand to get the initial condition  $\omega \rightarrow 1$  as  $z \rightarrow -\infty$  or equivalently  $x \rightarrow 0$ . In terms of this new variable  $z$ , the full form of Thomas-Fermi-Dirac equation is then given by

$$(D^2 - 2D + 1)\omega(z) = \exp(3z) \left( \omega^{\frac{1}{2}} \exp\left(-\frac{z}{2}\right) + \alpha \right)^2 = F(z) \quad (60)$$

To obtain the particular integral, we follow the iterative technique. On the right hand side of the above equation we put the value of complementary function for  $\omega$  which we call as the zeroth iteration term and obtain the equation

$$(D^2 - 2D + 1)\omega(z) = F_0(z) \quad (61)$$

Defining  $(D - 1)\omega = u$ , then

$$\frac{du}{dz} - u = F_0(z) \quad (62)$$

where

$$F_0(z) = \exp(3z)[\{(A + Bz) \exp(z) + 1\}^{1/2} \exp(-z/2) + \alpha]^2$$

Hence using the standard technique of integrating factor, which in this case is  $\exp(-z)$ , we have

$$u(z) = \exp(z)(F_1(z)) \quad (63)$$

where

$$F_1(z) = \int_{-\infty}^z \exp(2z')[\{(A + Bz') \exp(z')\}^{1/2} \exp(-z'/2) + \alpha]^2 dz' \quad (64)$$

Here to obtain the complete solution, we demand that  $\exp(-z)u \rightarrow 0$  as  $z \rightarrow -\infty$ . Using the same integrating factor technique, one can solve the equation

$$\frac{d\omega}{dz} - \omega = \exp(z)F_1(z) \quad (65)$$

Hence the complete solution is

$$\omega(z) = \exp(z)(A + Bz) + 1 + \exp(z) \int_{-\infty}^z F_1(z') dz' \quad (66)$$

Obviously  $\omega(z) \rightarrow 1$  as  $z \rightarrow -\infty$ . It can further be shown that the boundary condition in  $z$ -coordinate is given by

$$\left. \frac{d\omega}{dz} \right|_{z=z_s} = \omega(z) \big|_{z=z_s} \quad (67)$$

Then we have  $B = 1/x_s$ . We have used this value of  $B$  in the complete solution as given by eqn.(66). The constant  $A$  can be obtained numerically, provided the surface value  $x_s$  is known. Further, the surface value of scaled radius parameter and the constant  $A$  can be solved numerically using the expression for total number of electrons, given by

$$N = Z = \int d^2r n_e(r) \quad (68)$$

and eqn.(67). In  $x$ -coordinate eqn.(68) can be expressed as

$$N = Z = b \int_0^{x_s} dx \left\{ \frac{4\pi}{3m} b^{\frac{1}{2}} x^{\frac{1}{2}} + (2m)^{\frac{1}{2}} (Ze^2)^{\frac{1}{2}} \omega^{\frac{1}{2}} \right\}^2 \quad (69)$$

Here we have assumed that the number of electrons within the WS cell is equal to the number of protons within the nucleus situated at the centre of the cell. The WS cell is therefore charge neutral. As a consequence, the electric field at the surface vanishes exactly. We continue the iterative calculation for the particular integral, until the result converges. In fig.(2) we have plotted the variation of scaled surface radial parameter with the atomic number  $Z$ , which is also the number of electrons within the two-dimensional WS cell. It is obvious that the scaled parameter monotonically increases with  $Z$ . This type of variation can not be obtained in the case of Thomas-Fermi calculation. Therefore as we have noticed in the three-dimensional case, here also the WS cell has finite radius only in Thomas-Fermi-Dirac model.

## 5 Electron Exchange Energy for $B \neq 0$

In presence of a strong quantizing magnetic field the semi-analytical expression for exchange energy can be obtained for electrons assuming that all of them occupy only their zeroth Landau level. In this case the numerically fitted form of exchange energy is given by [9, 10]

$$U_{ex} = \alpha[1 - \exp(-\beta p_F)] \quad (70)$$

with the average values for  $\alpha \approx 5MeV$  and  $\beta \approx 1.5MeV^{-1}$  for the strength of magnetic field ranging from  $10^{13}G$  to  $10^{15}G$ . This range has special importance in the physics of strongly magnetized stellar electron gas. The Thomas-Fermi-Dirac condition is then given by

$$\mu = \frac{p_F^2}{2m} - e\phi - \alpha[1 - \exp(-\beta p_F)] \quad (71)$$

Hence one can obtained the numerically fitted form of Fermi momentum, given by

$$p_F = c(\mu^* + e\phi)^\nu \quad (72)$$

where the average values for  $c \approx 0.7$  and  $\nu \approx 0.5$  are for the same range of magnetic field. Here  $\mu^* = \mu + \alpha$ . Unfortunately, the Fermi momentum  $p_F$  here is along the third dimension, i.e, along  $z$  axis, which does not exist in this particular investigation. Hence we can conclude that exchange interaction term does not contribute when a 2D electron gas is placed in a strong magnetic field which populates only the zeroth Landau level for the electrons.

## 6 Appendix

To evaluate the kinetic pressure for degenerate electron gas in 2D in presence of strong quantizing magnetic field, we use the Euler summation formula as given bellow [21]

$$\sum_{j=0}^{\infty} f\left(j + \frac{1}{2}\right) \approx \int_0^{\infty} f(x)dx + \frac{1}{24}f'(0) \quad (73)$$

Then from eqn.(33) the q-potential can be re-written in presence of an electrostatic potential  $\phi$  in the following form

$$q = \sum_i \ln[1 + \exp(-\alpha' - \beta\varepsilon_i)] \quad (74)$$

where  $\alpha' = \alpha + \beta e\phi = \beta(-\mu - e\phi)$ . Hence

$$\begin{aligned} q &= \frac{SeB}{2\pi^2} \sum_{n=0}^{\infty} \ln \left[ 1 + \exp \left( -\alpha' - \beta \left( n + \frac{1}{2} \right) \omega \right) \right] \\ &= \frac{SeB}{2\pi^2} \left[ \int_0^{\infty} \ln[1 + \exp(-\alpha' - \beta x\omega)] dx - \beta\hbar\omega \frac{1}{\exp(\alpha') + 1} \right] \end{aligned} \quad (75)$$

After evaluating the integral by parts, we have

$$q = \frac{SeB}{2\pi} \beta\omega \left[ \int_0^{\infty} \frac{x dx}{\exp(\alpha' + \beta x\omega) + 1} - \frac{1}{\exp(\alpha') + 1} \right] \quad (76)$$

For  $T = 0$ , or  $T \ll T_F$ , where  $T_F$  is the Fermi temperature, given by  $\mu = T_F$ , for  $k_B = 1$ , the second term vanishes, whereas in the first part, putting the Fermi distribution = 1, the first part gives  $\mu'/2\omega$ , with  $\mu'^2 = \mu + e\phi$ . Then substituting the value of the integral in eqn.(76), we have

$$q = \beta PS = \frac{SeB}{4\pi^2} \beta \frac{1}{\omega} \mu'^2 \quad (77)$$

Hence

$$P(r) = \frac{m}{4\pi^2} (\mu + e\phi(r))^2 \quad (78)$$



## 7 Conclusion

It is quite surprising that the form of Thomas-Fermi differential equation in presence of strong quantizing magnetic field is exactly identical with that of zero field case. The exchange part of electron energy does not exist in 2D in presence of strong quantizing magnetic field. The Fermi momentum obtained in this case is along  $z$ -direction, which is suppressed in ideal 2D case. The Thomas-Fermi-Dirac equation therefore can not be obtained for a 2D electron gas in presence of a strong quantizing magnetic field. However, in absence of magnetic field, exchange energy can be obtained assuming a quasi 2D structure. Hence one can formulate Thomas-Fermi-Dirac model in 2D scenario for an electron gas. We have noticed that the radius of a two dimensional charge neutral WS cell is infinitely large. On the other hand it is finite if  $N/Z < 1$ , i.e., the cell is ionized or positively charged. In usual three dimensional case also the radius of an atom can not be finite in Thomas-Fermi model. However, in Thomas-Fermi-Dirac model the radius of a two dimensional charge neutral WS cell is found to be finite. We have also noticed that the size of circular shape WS cell does not depend on the strength of magnetic field, even if it is of astrophysical order. Because of two dimensional structure, there is no distortion of circular type WS cells to elliptical form. On the other hand, in the usual three dimensional case, because of pressure anisotropy within the WS cells, a distortion to ellipsoidal shape may occur in presence of strong quantizing magnetic field. In the usual three dimension, The anisotropy increases with the increase of the strength of magnetic field. Then in the extrim case, it can be shown that an atom becomes needle shape with its length alon the direction of magnetic field.

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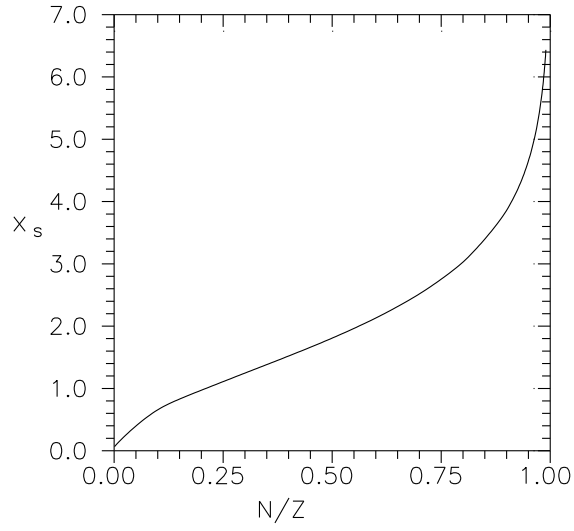


Figure 1: Variation of  $x_s$ , the scaled surface value of radius parameter with the ratio  $N/Z$

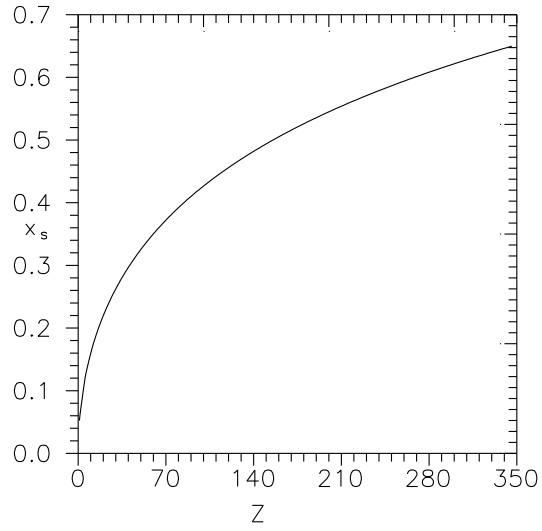


Figure 2: Variation of  $x_s$ , the scaled surface value of radius parameter with  $Z$

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